

# trans-Vaccenic acid, picolinyl ester

**Inchi:** InChI=1S/C24H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-24(26)27-22-23-18-  
**InchiKey:** UFDIVQGSXPHGEJ-BQYQJAHWSA-N  
**Formula:** C24H39NO2  
**SMILES:** CCCCCC=CCCCCCCCC(=O)OCc1cccnc1  
**Mol. weight [g/mol]:** 373.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.37		Crippen Method
logp	7.162		Crippen Method
mcvol	338.380	ml/mol	McGowan Method
rinsol	2874.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333558&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinsol:** Non-polar retention indices

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